

# Generalization Analysis for Unsupervised Nearest Neighbor Classification

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## Abstract

Learning a discriminative classifier from unlabeled data has been proven to be an effective way of simultaneously clustering the data and training a classifier from the data. We present a novel measure for evaluating the quality of a data partition by the misclassification rate of the nearest neighbor classifier learnt from that partition. By our unsupervised training scheme, we show the close relationship between the misclassification rate of the unsupervised nearest neighbor classifier and the widely used normalized graph Laplacian produced from isotropic kernel, and the misclassification rate reduces to the well-known kernel form of graph cut assuming uniform distribution. By minimizing the bound for the misclassification rate we also derive a new clustering algorithm, i.e. the Normalized Harmonic Cut (NHC). We show that that NHC is equivalent to normalized cut in case of uniform distribution, and our analysis provides an unified view of clustering and classification by evaluating the misclassification rate of the learnt classifier. Experimental results and comparisons with other clustering methods on real data sets demonstrate the effectiveness of the Normalized Harmonic Cut, which also shows the potential of our generalization analysis.

**Keywords:** Unsupervised Nearest Neighbor Classifier, Generalization Analysis

## 1. Introduction

Clustering methods partition the data into a set of self-similar clusters. Representative clustering methods include K-means (Hartigan and Wong, 1979) which minimizes the within-cluster dissimilarities, spectral clustering (Ng et al., 2001) which identifies clusters of more complex shapes lying on some low dimensional manifolds, and statistical modeling method (Fraley and Raftery, 2002) approximates the data by a mixture of parametric distribution. Although such clustering methods achieve promising result in practice, they ignore the inherent connection between the obtained clusters and the classes from supervised learning perspective. As a result, they not only lose a chance of potentially obtaining better data partitions, but also cannot utilize the effective tools from supervised learning community to produce data clusters which are also suitable for further classification.

Viewing clusters as classes, Recent works on unsupervised classification manage to learn a classifier from unlabeled data, and they have established the connection between clustering and multi-

class classification from a supervised learning perspective. (Xu et al., 2004) learns a max-margin two-class classifier in an unsupervised manner. Also, (Agakov and Barber, 2005) and (Gomes et al., 2010) learn the kernelized Gaussian classifier and the kernel logistic regression classifier respectively. Both (Gomes et al., 2010) and (Bridle et al., 1991) adopt the entropy of the posterior distribution of the class label by the classifier to measure the quality of the learnt classifier, and the parameters of such unsupervised classifiers can be computed by continuous optimization. More recent work presented in (Sugiyama et al., 2011) learns an unsupervised classifier by maximizing the mutual information between cluster labels and the data, and the Squared-Loss Mutual Information is employed to produce a convex optimization problem.

However, few methods consider the misclassification rate of the learnt classifier, one of the most important performance measures for classifiers, so that the performance of the unsupervised classifier is not fully evaluated by many methods. Although Bengio et al. (Bengio et al., 2003) analyzed the out-of-sample error for unsupervised learning algorithms, their method focused on lower-dimensional embedding of the data points and did not train a classifier from unlabeled data. In contrast, we learn the unsupervised nearest neighbor classifier (1-NN) from the data by our supervised training scheme introduced in the next section, and analyze the its misclassification rate on the  $\delta$ -cover of the data and the entire space. By minimizing the misclassification of 1-NN on the entire space, we design a new clustering method called Normalized Harmonic Cut (NHC). Our generalization analysis shows that the misclassification rate of 1-NN is closely related to widely used normalized graph Laplacian by isotropic kernel actually bounds the misclassification rate of 1-NN, and it is equivalent to the well-known graph cut (or unnormalized graph Laplacian) when the data points are sampled from a uniform distribution. Following this analysis it is shown that the NHC is equivalent to normalized cut (Shi and Malik, 2000) or Laplacian eigenmaps when the data points are mapped to one dimensional discrete label space in case of uniform distribution. Experimental results show the effectiveness of NHC over other clustering methods.

Although the generalization property of 1-NN have been extensively studied since (Cover and Hart, 1967), to the best of our knowledge most analysis focuses on the case where the training data are random. In this work, we propose to measure the quality of a specific data partition by the misclassification rate of 1-NN learnt from that partition, so we derive the misclassification rate of 1-NN with fixed training data (details in next section).

The rest part of this paper is organized as follows. We first introduce the formulation of unsupervised 1-NN classification in Section 2, then derive the misclassification rate of 1-NN and the Normalized Harmonic Cut algorithm in Section 3. After that, we demonstrate and analyze the experimental results, and finally conclude the paper.

## 2. Formulation of Unsupervised Nearest Neighbor Classification

Before formulating our clustering method, we introduce the notations in the formulation of unsupervised classification by nearest neighbor classifier. Suppose we are given the data set  $\tilde{X} = \{x_i\}_{i=1}^N \subset R^D$ , the goal of clustering is to find the cluster assignments  $\tilde{Y} = (y_1, y_2, \dots, y_N)$  to the data, where  $y_i$  is the cluster label for  $x_i$ ,  $y_i \in \{1, 2, \dots, Q\}$  and  $Q$  is the number of clusters. We model clustering as a data partition problem, and the clustering algorithm partitions  $X$  into  $Q$  disjoint clusters

$$C = \{C_i\}_{i=1}^Q, \text{ and } \tilde{X} = \bigcup_{i=1}^Q C_i.$$

## 2.1 Unsupervised Training Scheme

With any hypothetical data partition  $C$ , we can build the corresponding training data set  $S_C \triangleq \{(C_i, i)\}_{i=1}^Q$ , where  $i$  is the class label for class  $C_i$ , for a potential classifier. Note that such unsupervised training process exhibits combinatorics property, and the number of data partitions (the bell number  $B_N$ ) is prohibitively large in case that  $Q$  is unknown. In this way, the quality of a data partition can be evaluated by the performance of the classifier learnt from that partition. Since the training error of 1-NN is always zero, the misclassification rate of the nearest neighbor classifier associated with a data partition is considered instead, and we prefer the data partition with minimal associated misclassification rate.

It is worthwhile to mention that previous unsupervised classification methods (Sugiyama et al., 2011; Gomes et al., 2010) circumvent the above combinatorial unsupervised training scheme by learning a probabilistic classifier from the whole data, so they can not evaluate the classification performance of the learnt classifier. (Xu et al., 2004) learns the max-margin classifier by the combinatorial training scheme and minimized its misclassification rate, however, they can not handle the case that the number of classes  $Q$  is unknown. On the contrary, starting from the analysis of the misclassification rate of 1-NN, we derive a novel density-based cut function which only involves pairwise interactions between data points and does not depend on  $Q$ . Our new measure can be equipped either with a normalization step to handle fixed number of classes, resulting in a new Normalized Harmonic Cut algorithm superior to traditional normalized cut in the experimental result, or the exemplar-based clustering scheme (Frey and Dueck, 2007) to automatically determine the number of clusters by model selection.

## 2.2 The misclassification rate

Suppose  $(X, Y)$  are random variables indicating unobserved data point and its class label respectively,  $(X, Y) \in \mathcal{X} \times \mathcal{Y}$ , and  $\mathcal{D}$  is the distribution over  $\mathcal{X} \times \mathcal{Y}$ . We then denote by  $\mathbb{E}_{S_C, R_X}$  the misclassification rate of the 1-NN learnt from the training data  $S_C$  with a loss function  $L$  (Bishop, 2006):

$$\mathbb{E}_{S_C} = \mathbb{E}_{(X, Y) \sim \mathcal{D}, X \in \mathcal{X}} [L(Y, NN_{S_C}(X)) | S_C] \quad (1)$$

$$L(i, j) = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{otherwise} \end{cases}$$

Also, the misclassification rate constrained on  $R_X \subseteq \mathcal{X}$  is defined accordingly:

$$\mathbb{E}_{S_C, R_X} \triangleq \mathbb{E}_{(X, Y) \sim \mathcal{D}, X \in R_X} [L(Y, NN_{S_C}(X)) | S_C] \quad (2)$$

And we prefer the data partition with minimal associated misclassification rate  $\mathbb{E}_{S_C}$ . In our analysis  $\mathcal{Y} = \{1, 2, \dots, Q\}$ ,  $\mathcal{X}$  is bounded by  $[-M_0, M_0]^D$ ,  $\mathcal{D}_X$  is the induced marginal distribution over  $\mathcal{X}$ . We suppose that the data  $\tilde{X} = \{x_i\}_{i=1}^N$  are sampled i.i.d. from  $\mathcal{D}_X$ , and  $NN_S(X)$  is the classification function which returns the class label of a sample  $X$  by the 1-NN rule learnt from  $S$ . We also let  $f$  be the density function of  $\mathcal{D}_X$ ,  $\eta_i(x)$  be the posterior distribution of  $X = x$  over the labels, i.e.  $\eta_i(x) = P[Y = i | X = x]$ , and  $(f_j, \pi_j)$  be the density function and prior for class  $j$ . It is further assumed that  $f$  and  $\{\eta_i\}_{i=1}^Q$  satisfy the following two conditions:

A)  $f$  is bounded, i.e.  $f_{\min} \leq f \leq f_{\max}$ .

B) Both  $f$  and  $\{\eta_i\}_{i=1}^Q$  are Lipschitz:  $|f(x) - f(y)| \leq c \|x - y\|$ ,  $|\eta_i(x) - \eta_i(y)| \leq c_i \|x - y\|$  where  $c$  and  $\{c_i\}_{i=1}^Q$  are the corresponding Lipschitz constant.

In the following text we abbreviate  $S_C$  to  $S$ .

### 3. Clustering by Unsupervised Nearest Neighbor Classification

#### 3.1 Generalization Analysis for the 1-NN Trained with Given Data

We start the generalization analysis of the 1-NN constrained on the  $\delta$ -cover of the data  $\tilde{X}$  first, since the decision regions under the 1-NN rule can be easily constructed on the  $\delta$ -cover. It is interesting to observe that the constrained misclassification error of 1-NN is closely related to graph cut by the isotropic kernel.

**Definition 1** The  $\delta$ -cover of the data  $\tilde{X}$  is defined as  $B_\delta \triangleq \{B(x_m, \delta)\}_{m=1}^N$ , where  $B(x_m, \delta)$  is a ball centered at  $x_m$  with radius  $\delta > 0$ , and  $B(x_l, \delta) \cap B(x_m, \delta) = \emptyset$  for any  $l \neq m$ .

Suppose  $\mathcal{R}_{i,S}$  is the decision region for class  $i$  under the 1-NN rule trained from  $S$ , then it can be verified that  $\bigcup_{x_m \in C_i} B(x_m, \delta) \subseteq \mathcal{R}_{i,S}$ . Since the  $\delta$ -cover is comprised of the subsets of the decision regions, namely  $\bigcup_{i=1}^Q \bigcup_{x_m \in C_i} B(x_m, \delta) = B_\delta$ , we can derive the generalization properties of the 1-NN on the  $\delta$ -cover  $B_\delta$  by Theorem 2. Because we will estimate the underlying probabilistic density function (e.g.  $f$  and  $f_j$ ) frequently in the following text, we introduce the non-parametric kernel density estimator for  $f_j$  and  $f$  as below:

$$\hat{f}_j = \frac{1}{|C_j|} \sum_{x_l \in C_j} K_h(x - x_l) \quad \hat{f} = \frac{1}{N} \sum_{l=1}^N K_h(x - x_l) \quad (3)$$

where

$$K_h(x) = \frac{1}{(2\pi h^2)^{D/2}} e^{-\frac{\|x\|^2}{2h^2}} \quad (4)$$

is the isotropic Gaussian kernel with bandwidth  $h$  (Silverman, 1986), and we use  $\hat{\pi}_j = \frac{|C_j|}{N}$  as an estimator for  $\pi_j$ . Extensive study proves that the kernel density estimator (3) uniformly converges to the underlying density almost surely, as summarized in (Wied and Weißbach, 2010).

**Theorem 2 1.** The misclassification rate (2) of the 1-NN rule constrained on the  $\delta$ -cover of the data  $\tilde{X}$  in terms of the class-conditional density functions and priors is

$$\mathbb{E}_{S, B_\delta} = \sum_{i=1}^Q \sum_{j \neq i} \int_{\bigcup_{x_m \in C_i} B(x_m, \delta)} f_j(x) \pi_j dx \quad (5)$$

2. The estimator for  $\mathbb{E}_{S, B_\delta}$  using  $\{\hat{f}_j, \hat{\pi}_j\}_{j=1}^Q$  is given by

$$\hat{\mathbb{E}}_{S, B_\delta} = \frac{1}{N} \sum_{l,m=1}^N \theta_{lm} \int_{B(x_m, \delta)} K_h(x - x_l) dx \quad (6)$$

and

$$\left| \frac{\widehat{\mathbb{E}}_{S, B_\delta}}{\delta^D} - \sum_{l,m=1}^N \theta_{lm} K_h(x_m - x_l) \right| \leq \sum_{l,m=1}^N \theta_{lm} M \delta^2 \quad (7)$$

where  $M = \frac{c_0 D}{(2\pi)^{\frac{D}{2}} h^{D+2} (D+2)}$  and  $c_0$  is the volume of the unit ball in  $R^D$ ,  $\theta_{lm}$  is a class indicator function such that  $\theta_{lm} = 1$  if  $x_l, x_m$  belongs to different classes in  $S$  and 0 otherwise.

**Proof 1.**

$$\begin{aligned} \mathbb{E}_{S, B_\delta} &= \mathbb{E}_{X \in B_\delta} [\mathbb{E}_Y [L(Y, NN_S(X)) | S, X]] \\ &= \mathbb{E}_{X \in B_\delta} [P[Y \neq NN_S(X) | S, X]] \\ &= \sum_{i=1}^Q \mathbb{E}_{X \in \bigcup_{x_m \in C_i} B(x_m, \delta)} [P[Y \neq i | X]] \\ &= \sum_{i=1}^Q \sum_{j \neq i} \int_{\bigcup_{x_m \in C_i} B(x_m, \delta)} f_j(x) \pi_j dx \end{aligned}$$

2. It can be proved by expanding the kernel function by the second-order Taylor series. ■

The function  $\sum_{l,m=1}^N \theta_{lm} K_h(x_m - x_l)$  in (7) is actually the graph cut function produced by isotropic kernel which is widely used in clustering and segmentation since (Wu and Leahy, 1993) and (Weiss, 1999), and we can see that this graph cut function bounded the constrained misclassification rate  $\mathbb{E}_{S, B_\delta}$  (normalized by  $\delta^D$ ) from (7). Also,

$$\lim_{\delta \rightarrow 0} \frac{\widehat{\mathbb{E}}_{S, B_\delta}}{\delta^D} = \sum_{l,m=1}^N \theta_{lm} K_h(x_m - x_l)$$

Therefore, minimizing the above cut function also enforces the minimization of  $\mathbb{E}_{S, B_\delta}$  normalized by  $\delta^D$  when  $\delta$  is small enough. We regard this as a connection between unsupervised min-cut and the bound for the misclassification rate of 1-NN. Since small  $\delta$  undermines the influence of non-uniform distribution on the misclassification rate, and the misclassification rate is originally defined on the entire space, we extend our analysis and consider its misclassification rate on the entire space  $\mathcal{X}$  to further exploit the generalization ability of 1-NN.

Since 1-NN rule makes hard decision for a given datum, we introduce the following soft NN cost function which converges to the 1-NN classification function, which is similar to the one adopted by Neighbourhood Components Analysis (Goldberger et al., 2004):

**Definition 3** *The soft 1-NN cost function is defined as*

$$\widetilde{NN}_{h^*, S}(x, i) = \frac{\sum_{l=1}^N K_{h^*}(x - x_l) \mathcal{I}_{C_i}(x_l)}{\sum_{l=1}^N K_{h^*}(x - x_l)} \quad (8)$$

where  $\widetilde{NN}_{h^*,S}(x, i)$  represents the probability that the datum  $x$  is assigned to class  $i$  by 1-NN learnt from  $S$ , and  $\mathcal{I}$  is an indicator function.

Then we have

**Theorem 4** *The misclassification rate of the 1-NN trained with fixed training data  $S$  is given by*

$$\mathbb{E}_S = \lim_{h^* \rightarrow 0} \mathbb{E}_{S, h^*} \quad (9)$$

where

$$\mathbb{E}_{S, h^*} = \sum_{i, j=1, \dots, Q, i \neq j} \mathbb{E}_X \left[ \eta_i(X) \widetilde{NN}_{h^*, S}(X, j) \right] \quad (10)$$

Theorem 4 explicitly gives the expression for the misclassification rate of the 1-NN trained with fixed training data  $S$ . In order to apply it in real problems, it is particularly important to derive the bound for the misclassification rate (9). Theorem 5 shows that, with a large probability, (10) is bounded by a new cut function:

**Theorem 5** *With probability greater than  $1 - 2Re^{-M_{h^*}}$ , the misclassification rate of the 1-NN evaluated at  $h^*$ , i.e.  $\mathbb{E}_{S, h^*}$ , satisfies:*

$$\begin{aligned} & \frac{1}{N} \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \int_{\mathcal{X}} \frac{\pi_i f_i(x) K_{h^*}(x - x_l)}{f(x) + \tilde{\varepsilon}} dx \leq \mathbb{E}_{S, h^*} \\ & \leq \frac{1}{N} \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \int_{\mathcal{X}} \frac{\pi_i f_i(x) K_{h^*}(x - x_l)}{f(x) - \tilde{\varepsilon}} dx \end{aligned} \quad (11)$$

where  $M_{h^*} = -2N(2\pi)^D h^{*2D} \varepsilon^2$ ,  $\tilde{\varepsilon} = (T_{h^*}^{(1)} + c) \sqrt{D} \tau + \varepsilon + T_{h^*}^{(2)}$ ,  $T_{h^*}^{(1)}, T_{h^*}^{(2)}, \varepsilon > 0$ ,  $T_{h^*}^{(1)} = \frac{1}{e^{1/2}(2\pi)^{D/2} h^{*D+1}}$ ,  $\lim_{h^* \rightarrow 0} T_{h^*}^{(2)} = 0$ ,  $h^*, \tau, \varepsilon$  are small enough such that  $\tilde{\varepsilon} < f_{\min}$ .  $c$  is the Lipschitz constant for the density function  $f$ .

Theorem 5 provides bounds on the misclassification rate evaluated at  $h^*$ , i.e.  $\mathbb{E}_{S, h^*}$ . By Theorem 4, we further analyze the asymptotic case when  $h^* \rightarrow 0$  in the following theorem, where a sequence  $\{h_N^*\}_{N=1}^\infty$  converging to zero is constructed and the limit for the associated error sequence  $\{\mathbb{E}_{S, h_N^*}\}_{N=1}^\infty$  is bounded.

**Theorem 6** *Let  $\{h_N^*\}_{N=1}^\infty$  be a sequence such that  $\lim_{N \rightarrow \infty} h_N^* = 0$  and  $h_N^* \geq N^{-d}$  with  $d < \frac{1}{2D}$ . When  $N \rightarrow \infty$ , then with probability 1,*

$$\frac{1}{N} \mathbb{E}_S^{\text{lower}} \leq \mathbb{E}_{S, h_N^*} \leq \frac{1}{N} \mathbb{E}_S^{\text{upper}} \quad (12)$$

$$\mathbb{E}_S^{\text{upper}} = \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \frac{\pi_i f_i(x_l)}{f(x_l) - \lambda_0 \tau_0 - \varepsilon} \quad (13)$$

$$\mathbb{E}_S^{\text{lower}} = \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \frac{\pi_i f_i(x_l)}{f(x_l) + \lambda_0 \tau_0 + \varepsilon} \quad (14)$$

where  $\lambda_0 > 0$  is a constant,  $\tau_0, \varepsilon > 0$  such that  $\lambda_0 \tau_0 + \varepsilon < f_{\min}$ .

By Theorem 6, the bound for the misclassification rate of 1-NN is faithfully obtained when the number of training samples goes to infinity. The asymptotic analysis presented by (12) can also be reasonably applied to estimate the misclassification rate of 1-NN trained with finite training samples, especially in case of large training data. Similar to Theorem 2, we use kernel density estimators  $\{\hat{f}_j, \hat{\pi}_j\}_{j=1}^Q$  by (3) to estimate the underlying class-conditional density functions and class priors, which results in the estimator for the upper bound in (12) as below (we neglect the constant factor  $1/N$ ) here:

$$\begin{aligned}\hat{\mathbb{E}}_S^{upper} &= \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \frac{\hat{\pi}_i \hat{f}_i(x_l)}{\hat{f}(x_l) - \lambda_0 \tau_0 - \varepsilon} \\ &= \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \frac{\frac{1}{N} \sum_{m=1}^N K_h(x_l - x_m) \mathcal{I}_{C_i}(x_m)}{\frac{1}{N} \sum_{k=1}^N K_h(x_l - x_k) - \lambda_0 \tau_0 - \varepsilon} \\ &= 2 \sum_{l < m} \theta_{lm} H_{lm}\end{aligned}\tag{15}$$

$$H_{lm} \triangleq \frac{K_h(x_l - x_m)}{Hmean(KS_l, KS_m)}$$

(15) is a cut function where  $Hmean(\cdot, \cdot)$  indicates the harmonic mean of two numbers, and  $KS_t$  is defined as  $KS_t = \sum_{k=1}^N K_h(x_t - x_k) - N(\lambda_0 \tau_0 + \varepsilon)$  for any  $x_t \in \tilde{X}$ . In order to maximize the probability with which (11) holds, we prefer larger  $\tau$  (also  $\tau_0$ ) and larger  $\varepsilon$ , so that  $\lambda_0 \tau_0 + \varepsilon$  should be maximized. Since  $\frac{1}{N} K_h(0) < \frac{1}{N} \sum_{k=1}^N K_h(x_t - x_k)$  for every  $t$  (the lower bound is tight when  $h$  is small enough) and the inequality  $\lambda_0 \tau_0 + \varepsilon < \frac{1}{N} \sum_{k=1}^N K_h(x_t - x_k)$  should hold for any  $1 \leq t \leq N$ , we take  $\lambda_0 \tau_0 + \varepsilon = \frac{1}{N} K_h(0)$ , and the resultant cut is

$$H_{lm} = \frac{K_h(x_l - x_m)}{Hmean\left(\sum_{k=1, k \neq l}^N K_h(x_l - x_k), \sum_{k=1, k \neq m}^N K_h(x_m - x_k)\right)}\tag{16}$$

We call (16) harmonic cut since it involves the harmonic mean of two kernel sums. The harmonic cut function (15) is the kernel density estimator of the asymptotic bound for the misclassification rate of the 1-NN, and we need to minimize it following our clustering criteria in Section 2.

### 3.2 Minimizing the Misclassification Rate by NHC

Based on the analysis before, we design a clustering algorithm which minimizes the asymptotic bound for the misclassification rate of the 1-NN, so the objective function for our clustering algorithm in terms of kernel density estimator is actually the harmonic cut function (15). Written in a

matrix form, (15) is equivalent to  $\text{Tr}(Y^T LY)$  where  $Y = [Y_1 \ Y_2 \dots \ Y_Q]$  and each  $Y_i$  is a column vector of length  $N$  such that  $Y_{ik} = 1$  if  $x_k \in C_i$  and  $Y_{ik} = 0$  otherwise. We define  $\widehat{W} = [\widehat{w}_{ij}]_{N \times N}$  where  $\widehat{w}_{ij} = H_{ij}$  by (16), the diagonal matrix  $\widehat{D}$  where  $\widehat{D}_{ii} = \sum_{j=1}^N \widehat{w}_{ij}$ , and  $L = \widehat{D} - \widehat{W}$ . It can be verified that

$$\widehat{\mathbb{E}}_S^{\text{upper}} = 2 \sum_{l < m} \theta_{lm} H_{lm} = \text{Tr}(Y^T LY)$$

Therefore, the formulation of our clustering algorithm is below (we relax  $Y$  to take real values):

$$\min_{Y^T DY = I} \text{Tr}(Y^T LY) \quad (17)$$

where  $D$  is a diagonal matrix where  $D_{ii} = \sum_{j=1}^N w_{ij}$  is the sum of the elements of the  $i$ -th row of  $W = [w_{ij}]$ , and  $w_{ij} = K_h(x_i - x_j)$  by the isotropic kernel  $K_h$ . Similar to the Laplacian eigenmaps (Belkin and Niyogi, 2003), the constraint  $Y^T DY = I$  removes the scaling factor when minimizing (17) with respect to  $Y$ . Note that  $\widehat{W} = D^{-1}W + (D^{-1}W)^T$  which can be represented in terms of normalized graph Laplacian<sup>1</sup>. Moreover, if  $\mathcal{D}_{\mathcal{X}}$  is a uniform distribution,  $f$  is a constant and hence we do not need  $\widehat{f}$  as an estimator for  $f$  in (15), and  $\widehat{W} = W$  (up to a constant factor) which is the graph cut function produced by the isotropic kernel. In this case, we can see that (17) is equivalent to normalized cut (Shi and Malik, 2000).

Following the method for Rayleigh quotient (Golub and van Van Loan, 1996), (17) is minimized by solving the generalize eigenvalue system shown in Algorithm 1. It should be emphasized that unlike normalized cut where the isotropic kernel matrix  $W = [K_h(x_l - x_m)]$  is used to measure the affinity between data points, we employ the harmonic cut  $\widehat{W} = [H_{lm}]$  as the affinity measure. Note that the implementation of Algorithm 1 is quite similar to that of normalized cut, and the optimization is performed efficiently by solving a generalized eigenvector problem.

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**Algorithm 1** Normalized Harmonic Cut (NHC)
 

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- 1:  $\tilde{X}$ : the data set for clustering,  $Q$ : the number of clusters;
  - 2: Calculate the harmonic cut matrix  $\widehat{W} = [\widehat{w}_{ij}]_{N \times N}$  by (16) where  $\widehat{w}_{ij} = H_{ij}$ , and the diagonal matrix  $\widehat{D}$  where  $\widehat{D}_{ii} = \sum_{j=1}^N \widehat{w}_{ij}$ .
  - 3: Compute the similarity matrix  $W = [w_{ij}]_{N \times N}$  where  $w_{ij} = K_h(x_i - x_j)$ , and the diagonal matrix  $D$  where  $D_{ii} = \sum_{j=1}^N w_{ij}$ .
  - 4: Compute the unnormalized Laplacian matrix  $L = \widehat{D} - \widehat{W}$ .
  - 5: Compute the first  $Q$  generalized eigenvectors for  $Lt = \lambda Dt$
  - 6: Denote the obtained  $Q$  eigenvectors by  $Y = [Y_1 \ Y_2 \dots \ Y_Q]$ , perform  $k$ -means clustering on the rows of  $Y$ . Suppose the cluster label for the  $i$ -th row is  $y_i$ ,  $1 \leq i \leq N$ .
  - 7: Assign the cluster label  $y_i$  to data point  $x_i$ ,  $1 \leq i \leq N$ .
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#### 4. Connection to Existing Methods

Derived from the bound for the misclassification rate of the 1-NN, the harmonic cut exhibits interesting similarity to existing cut-based clustering methods. The graph cut function  $\sum_{l,m=1}^N \theta_{lm} K_h(x_m - x_l)$

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1. Normalized graph Laplacian is  $\widehat{L} = I - D^{-1}W$  and  $\widehat{W}$  is related to  $\widehat{L}$  by  $\widehat{W} = 2I - \widehat{L} - \widehat{L}^T$



has been extensively used for clustering and segmentation by (Wu and Leahy, 1993; Weiss, 1999; Shi and Malik, 2000; Ng et al., 2001; Luxburg, 2007), which also bounds the misclassification rate of 1-NN on the  $\delta$ -cover and on the entire space in case of uniform distribution. Such graph cut function easily produces imbalanced data partitions, and normalized cut (Shi and Malik, 2000) solves this problem by introducing a normalization factor in the cut function which controls the cluster size and obtains more desirable results. It should be emphasized that all these methods heavily rely on the pairwise similarity or affinity matrix  $W$  which encodes the affinity between data points, and two data points are more likely to be assigned to different clusters if the affinity between them is low. In contrast to the cut function by isotropic Gaussian kernel, the harmonic cut function used in NHC is built upon the generalization analysis of unsupervised 1-NN classification, which shows advantages over other cut-based clustering methods in real data sets. As mentioned in previous section, normalized cut becomes a special case of NHC assuming uniform distribution. Moreover, the harmonic cut (16) is similar to the row-normalized kernel for building the diffusion map (Coifman et al., 2005; Coifman and Lafon, 2006), which is used to account for the influence of non-uniform distribution on the affinity function. Similar to normalized cut (Shi and Malik, 2000) or spectral clustering (Ng et al., 2001), NHC is efficient since it only requires solving a eigenproblem shown in Algorithm 1.

NHC is also closely related to the cut function in (Narayanan et al., 2006). In this work, the data  $\tilde{X}$  lies on a domain  $\Omega \subseteq R^D$ . Suppose  $p$  is the probability density function on  $\Omega$  and  $S$  is the boundary which separate  $\Omega$  into two parts. Let  $X_1$  and  $X_2$  be the partition of  $\tilde{X}$  by  $S$ . Then the authors provide the asymptotic analysis proving that the following cut function

$$\frac{1}{N} \sqrt{\frac{2\pi}{h_N}} \sum_{x_l \in X_1} \sum_{x_m \in X_2} V_{lm} \quad (18)$$

converges to the volume of the class boundary  $S$ , i.e.  $\int_S p(s)ds$ , where  $Gmean(\cdot, \cdot)$  is the geometric mean of two numbers and  $V$  is defined as

$$V_{lm} \triangleq \frac{K_{h_N}(x_l - x_m)}{Gmean\left(\sum_{k \neq l} K_{h_N}(x_l - x_k), \sum_{k \neq m} K_{h_N}(x_m - x_k)\right)} \quad (19)$$

Compared to the harmonic cut (16), we observe that  $H_{lm} \geq V_{lm}$  when  $h = h_N$  by Cauchy-Schwarz inequality. So that harmonic cut is the tight upper bound for the cut (19) given a fixed kernel bandwidth, and the latter eventually converges to  $\int_S p(s)ds$  (multiplied by a term  $\sqrt{\frac{2\pi}{h_N}}$ ). According to the widely accepted Low Density Separation assumption stating that the class boundary tends to pass through regions of low density, the low  $\int_S p(s)ds$  is preferred. Minimizing the harmonic cut actually follows this principle.

## 5. Experimental Results

While our main contribution focuses on the derivation of the generalization ability for unsupervised 1-NN classification, we derive the NHC algorithm based on our generalization analysis and show its performance in real data sets in this section.

Since the formulation of NHC is derived from graph cut perspective, so the NHC algorithm falls into the category of clustering methods based on cut, and we compare NHC to Normalized Cut (NC) (Shi and Malik, 2000) and K-means. NHC is also compared to spectral clustering (SC) (Ng et al., 2001), since Shi’s NC and Ng’s SC are actually two versions of normalized spectral clustering.

We use the popular adjusted rand index (ARI) (Hubert and Arabie, 1985) for evaluating the performance of the clustering methods. ARI is the adjusted-for-chance version of rand index, and it has been widely used as a measure of agreement between the inferred cluster labels and the ground truth cluster assignments. ARI ranges from  $-1$  to  $1$ , and it achieves the maximum  $1$  when the inferred label is identical to the ground truth. A higher ARI indicates a better agreement between the inferred data partition and the ground truth partition.

The input data set is centralized and its variance is normalized in each dimension (with unit variance) before we feed it into clustering methods. We apply K-means, Spectral Clustering, Normalized Cut and Normalized Harmonic Cut to three UCI repository (Vertebral Column, Breast Tissue, SPECT Heart). We choose the kernel bandwidth  $h$  in the kernel density estimator (16) as  $h = \alpha Dist_{\max}$ , where  $Dist_{\max}$  is the maximum squared distance between data points, and  $\alpha$  is a bandwidth ratio. In our experiments we let  $\alpha$  range from  $0.01$  to  $0.2$  to see the performance change of various clustering methods. For a fair comparison SC, NC, and NHC share the same kernel bandwidth  $h$ . Since all the four clustering methods involve random initialization in the K-means step, we run them 50 times and take the average. The clustering result is shown in Figure 1 and 2.

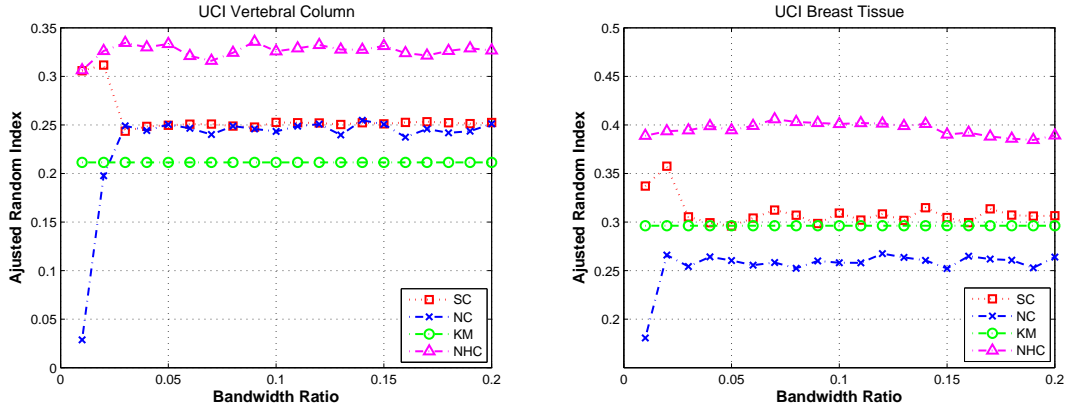


Figure 1: Clustering on UCI Vertebral Column and Breast Tissue Data Sets

As expected from our theoretical analysis, NHC always performs better than NC, and it also frequently renders better result than SC. We also observe that NHC is stable with varying kernel bandwidth.

## 6. Conclusion

Learning a classifier from unlabeled data is promising for both clustering and classification. We learn the nearest neighbor classifier from the data in an unsupervised manner, and analyze the its misclassification rate on the  $\delta$ -cover of the data and on the entire space. Our generalization analysis shows the close relationship between the widely used graph Laplacian produced by isotropic kernel

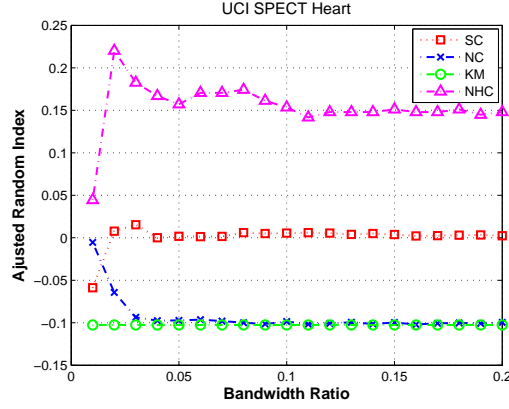


Figure 2: Clustering on UCI SPET Heart Data Set

and the misclassification rate of 1-NN. We further obtain the asymptotic bound for the misclassification rate of 1-NN by kernel density estimation. A new clustering method, Normalized Harmonic Cut, is derived by minimizing such asymptotic misclassification bound. Effectiveness of NHC is evidenced by experiments on real UCI data sets.

## Appendix

**Proof [Proof of Theorem 4]** It can be verified that

$$\lim_{h^* \rightarrow 0} \widetilde{NN}_{h^*,S}(x, i) = P[NN_S(X) = i | X = x, S] \quad (20)$$

Similar to the proof of Theorem 2, we have

$$\begin{aligned} \mathbb{E}_S &= \mathbb{E}_{(X,Y)} [L(Y, NN_S(X)) | S] \\ &= \mathbb{E}_X [\mathbb{E}_Y [L(Y, NN_S(X)) | S, X]] \\ &= \mathbb{E}_X [P[Y \neq NN_S(X) | S, X]] \\ &= \mathbb{E}_X \left[ \sum_{i,j=1,\dots,Q, i \neq j} P[Y = i | X] P[NN_S(X) = j | X, S] \right] \\ &= \sum_{i,j=1,\dots,Q, i \neq j} \mathbb{E}_X [\eta_i(X) P[NN_S(X) = j | X, S]] \end{aligned} \quad (21)$$

since  $Y$  and  $NN_S(X)$  are conditionally independent given  $X$ . Also, the product  $\eta_i(X) \widetilde{NN}_{h^*,S}(X, j) \leq 1$ , based on (20) and the dominated convergence theorem, we get

$$\begin{aligned} &\lim_{h^* \rightarrow 0} \mathbb{E}_X [\eta_i(X) \widetilde{NN}_{h^*,S}(X, j)] \\ &= \mathbb{E}_X \left[ \lim_{h^* \rightarrow 0} \eta_i(X) \widetilde{NN}_{h^*,S}(X, j) \right] \\ &= \mathbb{E}_X [\eta_i(X) P[NN_S(X) = j | S, X]] \end{aligned} \quad (22)$$

Substituting (22) into (21), we finish the proof.  $\blacksquare$

Before the proof of Theorem 5, we introduce the following two lemmas:

**Lemma 7** *Suppose  $\mathcal{D}$  is a probabilistic distribution with density function  $f$  which satisfies the two conditions A and B in Section 2, then we have*

$$\forall z \in \mathcal{X} \quad \lim_{h^* \rightarrow 0} \int_{\mathcal{X}} f(x) K_{h^*}(x - z) dx = f(z) \quad (23)$$

where  $K$  is defined as a Gaussian kernel  $K_{h^*}(x) \triangleq \frac{1}{(2\pi h^{*2})^{D/2}} e^{-\frac{\|x\|^2}{2h^{*2}}}$ , and this convergence is uniform.

**Lemma 8** *The function*

$$T(x) \triangleq \sum_{i=1}^N K_{h^*}(x - x_i) \quad x_i \in \tilde{X} \quad (24)$$

is uniformly continuous, i.e.  $|T(x) - T(y)| \leq T_{h^*} \|x - y\|$  for any  $x, y \in \mathcal{X}$ , where  $T_{h^*} = \frac{N}{e^{1/2}(2\pi)^{D/2} h^{*D+1}}$ .

**Proof [Proof of Theorem 5]** Let  $\{P_1, P_2, \dots, P_R\}$  be the  $\tau$ -cover of the set  $\mathcal{X}$ . Suppose  $R$  points  $\{\hat{x}_r\}_{r=1}^R$  are chosen from  $\mathcal{X}$  and  $\hat{x}_r \in P_r$ . For each  $1 \leq r \leq R$ , according to the Hoeffding's inequality

$$\Pr \left[ \left| \frac{T(\hat{x}_r)}{N} - \mathbb{E}_Z [K_{h^*}(\hat{x}_r - Z)] \right| > \varepsilon \right] < 2e^{-M_{h^*}} \quad (25)$$

where  $T$  is defined in (24) and  $\mathbb{E}_Z [K_{h^*}(\hat{x}_r - Z)] = \int_{\mathcal{X}} f(z) K_{h^*}(\hat{x}_r - z) dz$ . By the union bound, the probability that the above event happens for  $\{\hat{x}_r\}_{r=1}^R$  is less than  $2Re^{-M_{h^*}}$ . It follows that with probability greater than  $1 - 2Re^{-2Nh^{*2D}\varepsilon^2}$ ,

$$\left| \frac{T(\hat{x}_r)}{N} - \mathbb{E}_Z [K_{h^*}(\hat{x}_r - Z)] \right| \leq \varepsilon \quad (26)$$

holds for any  $1 \leq r \leq R$ .

For any  $x \in \mathcal{X}$ ,  $x \in P_r$  for some  $P_r \in P$  where  $P$  is the  $\tau$ -cover of  $\mathcal{X}$ . By Lemma 8,

$$\begin{aligned} \frac{1}{N} |T(x) - T(\hat{x}_r)| &\leq \frac{T_{h^*}}{N} \|x - \hat{x}_r\| \leq \frac{T_{h^*}}{N} \sqrt{D}\tau \\ &= T_{h^*}^{(1)} \sqrt{D}\tau \end{aligned} \quad (27)$$

Also, since  $f$  is  $c$ -Lipschitz,

$$|f(x) - f(\hat{x}_r)| \leq c \|x - \hat{x}_r\| \leq c\sqrt{D}\tau \quad (28)$$

Moreover, by Lemma 7  $\lim_{h^* \rightarrow 0} \mathbb{E}_Z [K_{h^*}(\hat{x}_r - Z)] = f(\hat{x}_r)$  holds for any  $1 \leq r \leq R$  and this convergence is uniform, so there exists  $T_{h^*}^{(2)}$  such that

$$\begin{aligned} |\mathbb{E}_Z [K_{h^*}(\hat{x}_r - Z)] - f(\hat{x}_r)| &\leq T_{h^*}^{(2)} \\ \lim_{h^* \rightarrow 0} T_{h^*}^{(2)} &= 0 \end{aligned} \quad (29)$$

Combining (26) (27) (28) (29) we get

$$\left| \frac{T(x)}{N} - f(x) \right| \leq \left( T_{h^*}^{(1)} + c \right) \sqrt{D} \tau + \varepsilon + T_{h^*}^{(2)} \quad (30)$$

for any  $x \in \mathcal{X}$ . It is worthwhile to mention that we can always choose  $h^*, \tau, \varepsilon$  which are small enough so that  $\tilde{\varepsilon} < f_{\min}$  (e.g. choose  $\varepsilon < \frac{f_{\min}}{3}$  first, then choose  $h^*$  small enough such that  $T_{h^*}^{(2)} < \frac{f_{\min}}{3}$ , and choose  $\tau$  small enough to make  $\left( T_{h^*}^{(1)} + c\sqrt{D} \right) \tau < \frac{f_{\min}}{3}$ ). Note that

$$\begin{aligned} \mathbb{E}_{S, h^*} &= \sum_{i, j=1, \dots, Q, i \neq j} \mathbb{E}_X \left[ \eta_i(X) \widetilde{N N_{h^*, S}}(X, j) \right] \\ &= \sum_{i, j=1, \dots, Q, i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \int_{\mathcal{X}} \frac{\eta_i(x) K_{h^*}(x - x_l)}{T(x)} f(x) dx \\ &= \sum_{i, j=1, \dots, Q, i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \int_{\mathcal{X}} \frac{\pi_i f_i(x) K_{h^*}(x - x_l)}{T(x)} dx \end{aligned} \quad (31)$$

Then (11) follows by applying the inequality (30) to (31), when  $h^*, \tau, \varepsilon$  are small enough such that  $\tilde{\varepsilon} < f_{\min}$ .  $\blacksquare$

**Proof [Proof of Theorem 6]** By Theorem 5, with probability at least  $1 - 2Re^{-M_{h^*}}$ ,

$$\mathbb{E}_{S, h_N^*} \leq \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \int_P \frac{\pi_i f_i(x) K_{h_N^*}(x - x_l)}{N[f(x) - \tilde{\varepsilon}]} dx \quad (32)$$

when  $\tilde{\varepsilon} < f_{\min}$  where  $\tilde{\varepsilon} = \left( T_{h_N^*}^{(1)} + c \right) \sqrt{D} \tau_N + \varepsilon + T_{h_N^*}^{(2)}$ . Here we choose  $\tau_N = \tau_0 N^{-d(D+1)}$ . It can be obtained that

$$\tilde{\varepsilon} \leq \lambda_0 \tau_0 + \varepsilon + T_{h_N^*}^{(2)} + c \tau_0 \sqrt{D} N^{-d(D+1)} \quad (33)$$

where  $\lambda_0 = \sqrt{D} / \left[ e^{1/2} (2\pi)^{D/2} \right]$  and  $\tau_0$  is chosen such that  $\lambda_0 \tau_0 + \varepsilon + T_{h_N^*}^{(2)} + c \tau_0 \sqrt{D} N^{-d(D+1)} < f_{\min}$  for sufficiently large  $N$ . Note that  $\lim_{N \rightarrow \infty} T_{h_N^*}^{(2)} = \lim_{N \rightarrow \infty} c \tau_0 \sqrt{D} N^{-d(D+1)} = 0$ , after applying Lemma 7 we get

$$\lim_{N \rightarrow \infty} N \mathbb{E}_{S, h_N^*} \leq \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \frac{\pi_i f_i(x_l)}{f(x_l) - \lambda_0 \tau_0 - \varepsilon} \quad (34)$$

Following the similar argument

$$\lim_{N \rightarrow \infty} N \mathbb{E}_{S, h_N^*} \geq \sum_{i \neq j} \sum_{l=1}^N \mathcal{I}_{C_j}(x_l) \frac{\pi_i f_i(x_l)}{f(x_l) + \lambda_0 \tau_0 + \varepsilon} \quad (35)$$

Also, since  $R$  is the number of elements in the  $\tau$ -cover of  $\mathcal{X}$ ,  $R \leq \frac{(2M_0)^D}{\tau^D}$ . With the choice of  $\tau_N$ ,

$$\begin{aligned} & \lim_{N \rightarrow \infty} R e^{-M_h^*} \\ & \leq \lim_{N \rightarrow \infty} \frac{(2M_0)^D N^{dD(D+1)}}{\tau_0^D} e^{-2N^{1-2Dd}(2\pi)^D \varepsilon^2} = 0 \end{aligned} \quad (36)$$

Therefore, when  $N \rightarrow \infty$  (12) holds with probability 1. ■

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